Dimethyl succinate

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.93e-12 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 5.01e-01

Confidence level: 7.50e-01

Nearest Neighbors from the Training Set

Image not found
Dimethyl succinate
Measured: 1.40e-12
Predicted: 1.93e-12

Image not found
Dimethyl glutarate
Measured: 3.30e-12
Predicted: 3.76e-12

Image not found
Dimethyl adipate
Measured: 8.40e-12
Predicted: 6.84e-12

Image not found
Ethyl lactate
Measured: 3.90e-12
Predicted: 4.80e-12

Image not found
2-Ethoxyethyl acetate
Measured: 1.30e-11
Predicted: 1.03e-11